

Jądrowe funkcjonały gęstości

Jacek Dobaczewski
University of Warsaw & University of Jyväskylä

Współpracownicy w Jyväskylä:
Gillis Carlsson, Markus Kortelainen,
Kazuhito Mizuyama, Jussi Toivanen
(Rayner Rodriguez-Guzman)

Seminarium „Struktura jądra atomowego”

Uniwersytet Warszawski

16 kwietnia 2008



Plan seminarium

1. Podstawy teorii funkcjonału gęstości.
2. Jądrowy funkcjonał gęstości w postaci standardowej.
3. Zależność energii jednocząstkowych od stałych sprzężenia funkcjonału gęstości.
4. Dopasowania energii jednocząstkowych do danych doświadczalnych.
5. Dopasowania mas jądrowych – analiza i propagacja błędów w prostym modelu.
6. Podsumowanie i wnioski.

M. Kortelainen, J. Dobaczewski, K. Mizuyama, J. Toivanen, arXiv:0803.2291
submitted to Physical Review C

Hohenberg-Kohn theorem

For any many-fermion state $|\Psi\rangle$ one can determine spatial distribution of particles $\rho(\vec{r})$ in the following way:

$$\rho(\vec{r}) = \int d^3\vec{r}_1 \dots d^3\vec{r}_A \Psi^*(\vec{r}_1 \dots \vec{r}_A) \left(\sum_{i=1}^A \delta(\vec{r} - \vec{r}_i) \right) \Psi(\vec{r}_1 \dots \vec{r}_A).$$

This creates a map

$$|\Psi\rangle \longrightarrow \rho(\vec{r})$$

and defines the class of states $\{|\Psi\rangle\}_{\rho(\vec{r})}$ that all have the same density distribution

$$\rho(\vec{r}) \longrightarrow \{|\Psi\rangle\}_{\rho(\vec{r})}.$$

By minimizing the energy of the system within the class $\{|\Psi\rangle\}_{\rho(\vec{r})}$, we now define the energy-density-functional $\mathcal{E}[\rho(\vec{r})]$:

$$\mathcal{E}[\rho(\vec{r})] = \min_{\{|\Psi\rangle\}_{\rho(\vec{r})}} \langle \Psi | \hat{H} | \Psi \rangle.$$

It is then obvious that the exact ground-state energy E_0 is obtained by minimizing the functional $\mathcal{E}[\rho(\vec{r})]$ with respect to densities $\rho(\vec{r})$.

$$E_0 = \min_{\rho(\vec{r})} \mathcal{E}[\rho(\vec{r})].$$

Hohenberg-Kohn theorem (trivial version)

For any many-fermion state $|\Psi\rangle$ one can determine mean-square radius $\langle \vec{r}^2 \rangle$ in the following way:

$$\langle \vec{r}^2 \rangle = \int d^3\vec{r}_1 \dots d^3\vec{r}_A \Psi^*(\vec{r}_1 \dots \vec{r}_A) \left(\sum_{i=1}^A \vec{r}_i^2 \right) \Psi(\vec{r}_1 \dots \vec{r}_A).$$

This creates a map

$$|\Psi\rangle \longrightarrow \langle \vec{r}^2 \rangle$$

and defines the class of states $\{|\Psi\rangle\}_{\langle \vec{r}^2 \rangle}$ that all have the same mean-square radius

$$\langle \vec{r}^2 \rangle \longrightarrow \{|\Psi\rangle\}_{\langle \vec{r}^2 \rangle}.$$

By minimizing the energy of the system within the class $\{|\Psi\rangle\}_{\langle \vec{r}^2 \rangle}$, we now define the energy-density-functional $\mathcal{E}[\langle \vec{r}^2 \rangle]$:

$$\mathcal{E}[\langle \vec{r}^2 \rangle] = \min_{\{|\Psi\rangle\}_{\langle \vec{r}^2 \rangle}} \langle \Psi | \hat{H} | \Psi \rangle.$$

It is then obvious that the exact ground-state energy E_0 is obtained by minimizing the functional $\mathcal{E}[\langle \vec{r}^2 \rangle]$ with respect to mean-square radii $\langle \vec{r}^2 \rangle$:

$$E_0 = \min_{\langle \vec{r}^2 \rangle} \mathcal{E}[\langle \vec{r}^2 \rangle].$$

Nuclear Energy Density Functional (physical insight)

1° The energy-density functional that can be universal (valid for systems with any particle number) must depend at least on the local particle density:

$$\mathcal{E}'[\rho(\vec{r})] = \mathcal{E}[\rho(\vec{r})] - \lambda \int d^3\vec{r} \rho(\vec{r}).$$

2° The energy-density functional that can describe shell effects must depend on the local kinetic density (Kohn-Sham approach):

$$\mathcal{E}[\rho(\vec{r}), \tau(\vec{r})] = \frac{\hbar^2}{2m} \int d^3\vec{r} \tau(\vec{r}) + \mathcal{E}^{\text{int}}[\rho(\vec{r})].$$

3° The energy-density functional that can describe effective-mass, surface, and spin-orbit effects must in addition depend on the gradient of density and spin-momentum density:

$$\mathcal{E}[\rho(\vec{r}), \tau(\vec{r}), \vec{\nabla}\rho(\vec{r}), J_{\mu\nu}(\vec{r})] = \frac{\hbar^2}{2m} \int d^3\vec{r} \tau(\vec{r}) + \mathcal{E}^{\text{int}}[\rho(\vec{r}), \vec{\nabla}\rho(\vec{r}), J_{\mu\nu}(\vec{r})].$$

4° The energy-density functional that can describe time-odd effects must in addition depend on time-odd densities.

Nuclear Energy Density Functional

We consider the EDF in the form,

$$\mathcal{E} = \int d^3r \mathcal{H}(r),$$

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m} \tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta\rho_t + \frac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t.$$

Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters C_t^ρ on the isoscalar density ρ_0 as:

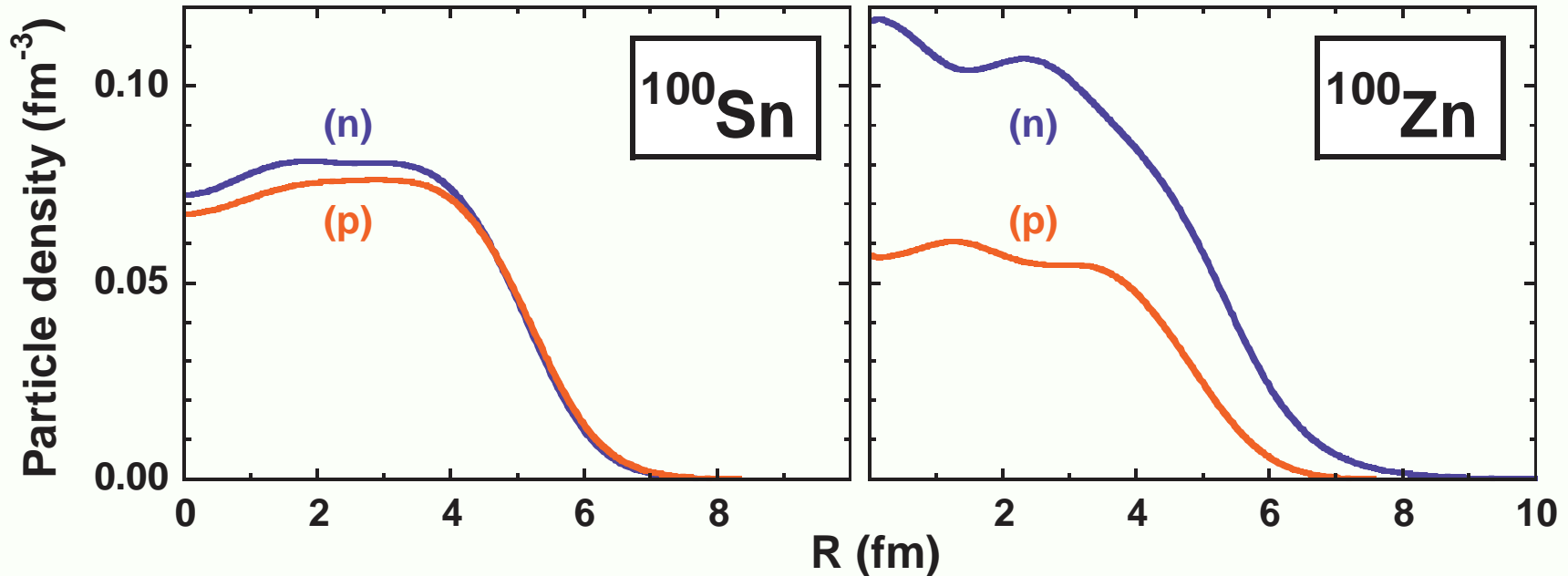
$$C_t^\rho = C_{t0}^\rho + C_{tD}^\rho \rho_0^\alpha.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{t0}^\rho, \quad C_{tD}^\rho, \quad C_t^\tau, \quad C_t^{\Delta\rho}, \quad C_t^J, \quad \text{and} \quad C_t^{\nabla J},$$

for $t = 0$ and 1.

Nuclear densities as composite fields



Modern Mean-Field Theory \equiv Energy Density Functional

ρ , τ , \vec{J} , \vec{j} , \vec{T} , \vec{S} , \vec{F} ,

- Hohenberg-Kohn
- Kohn-Sham
- Negele-Vautherin
- Landau-Migdal
- Nilsson-Strutinsky

mean field \Rightarrow one-body densities
 zero range \Rightarrow local densities
 finite range \Rightarrow non-local densities

Nuclear densities as composite fields

Density matrix:

$$\rho(\vec{r}\sigma, \vec{r}'\sigma') = \langle \Phi | a^\dagger(\vec{r}'\sigma') a(\vec{r}\sigma) | \Phi \rangle$$

Scalar and vector part:

$$\rho(\vec{r}, \vec{r}') = \sum_{\sigma} \rho(\vec{r}\sigma, \vec{r}'\sigma)$$

$$\vec{s}(\vec{r}, \vec{r}') = \sum_{\sigma\sigma'} \rho(\vec{r}\sigma, \vec{r}'\sigma') \langle \sigma' | \vec{\sigma} | \sigma \rangle$$

Symmetries:

$$\rho^T(\vec{r}, \vec{r}') = \rho^*(\vec{r}', \vec{r}) = \rho(\vec{r}', \vec{r})$$

$$\vec{s}^T(\vec{r}, \vec{r}') = -\vec{s}^*(\vec{r}', \vec{r}) = -\vec{s}(\vec{r}', \vec{r})$$

Local densities:

Matter:

$$\rho(\vec{r}) = \rho(\vec{r}, \vec{r})$$

Momentum:

$$\vec{j}(\vec{r}) = (1/2i)[(\vec{\nabla} - \vec{\nabla}')\rho(\vec{r}, \vec{r}')]_{r=r'}$$

Kinetic:

$$\tau(\vec{r}) = [\vec{\nabla} \cdot \vec{\nabla}' \rho(\vec{r}, \vec{r}')]_{r=r'}$$

Spin:

$$\vec{s}(\vec{r}) = \vec{s}(\vec{r}, \vec{r})$$

Spin momentum:

$$J_{\mu\nu}(\vec{r}) = (1/2i)[(\nabla_{\mu} - \nabla'_{\mu})s_{\nu}(\vec{r}, \vec{r}')]_{r=r'}$$

Spin kinetic:

$$\vec{T}(\vec{r}) = [\vec{\nabla} \cdot \vec{\nabla}' \vec{s}(\vec{r}, \vec{r}')]_{r=r'}$$

Tensor kinetic:

$$\vec{F}(\vec{r}) = \frac{1}{2}[(\vec{\nabla} \otimes \vec{\nabla}' + \vec{\nabla}' \otimes \vec{\nabla}) \cdot \vec{s}(\vec{r}, \vec{r}')]_{r=r'}$$

$$\mathcal{H}(r) = \frac{\hbar^2}{2m} \tau_0(r) + \sum_{t=0,1} \left(\overset{\text{p-h density}}{\chi_t(r)} + \overset{\text{p-p density}}{\check{\chi}_t(r)} \right)$$

Most general second order expansion in densities and their derivatives

$$\begin{aligned} \chi_0(r) = & C_0^{\rho} \rho_0^2 + C_0^{\Delta\rho} \rho_0 \Delta\rho_0 + C_0^{\tau} \rho_0 \tau_0 + C_0^{J_0} J_0^2 + C_0^{J_1} J_0^2 + C_0^{J_2} J_0^2 + C_0^{\nabla J} \rho_0 \nabla \cdot J_0 \\ & + C_0^s s_0^2 + C_0^{\Delta s} s_0 \cdot \Delta s_0 + C_0^T s_0 \cdot T_0 + C_0^j j_0^2 + C_0^{\nabla j} s_0 \cdot (\nabla \times j_0) + C_0^{\nabla s} (\nabla \cdot s_0)^2 + C_0^F s_0 \cdot F_0, \end{aligned}$$

$$\begin{aligned} \chi_1(r) = & C_1^{\rho} \vec{\rho}^2 + C_1^{\Delta\rho} \vec{\rho} \circ \Delta\vec{\rho} + C_1^{\tau} \vec{\rho} \circ \vec{\tau} + C_1^{J_0} \vec{J}^2 + C_1^{J_1} \vec{J}^2 + C_1^{J_2} \vec{J}^2 + C_1^{\nabla J} \vec{\rho} \circ \nabla \cdot \vec{J} \\ & + C_1^s \vec{s}^2 + C_1^{\Delta s} \vec{s} \circ \Delta\vec{s} + C_1^T \vec{s} \circ \vec{T} + C_1^j \vec{j}^2 + C_1^{\nabla j} \vec{s} \circ (\nabla \times \vec{j}) + C_1^{\nabla s} (\nabla \cdot \vec{s})^2 + C_1^F \vec{s} \circ \vec{F}, \end{aligned}$$

$$\begin{aligned} \check{\chi}_0(r) = & \check{C}_0^s |s_0|^2 + \check{C}_0^{\Delta s} \Re(\check{s}_0^* \cdot \Delta s_0) + \check{C}_0^T \Re(\check{s}_0^* \cdot T_0) \\ & + \check{C}_0^j |j_0|^2 + \check{C}_0^{\nabla j} \Re(\check{s}_0^* \cdot (\nabla \times j_0)) + \check{C}_0^{\nabla s} |\nabla \cdot s_0|^2 + \check{C}_0^F \Re(\check{s}_0^* \cdot F_0), \end{aligned}$$

$$\begin{aligned} \check{\chi}_1(r) = & \check{C}_1^{\rho} |\vec{\rho}|^2 + \check{C}_1^{\Delta\rho} \Re(\vec{\rho}^* \circ \Delta\vec{\rho}) + \check{C}_1^{\tau} \Re(\vec{\rho}^* \circ \vec{\tau}) \\ & + \check{C}_1^{J_0} |\vec{J}|^2 + \check{C}_1^{J_1} |\vec{J}|^2 + \check{C}_1^{J_2} |\vec{J}|^2 + \check{C}_1^{\nabla J} \Re(\vec{\rho}^* \circ \nabla \cdot \vec{J}). \end{aligned}$$

pairing
functional

- Not all terms are equally important. Usually ~12 terms considered
- Some terms probe specific experimental data
- Pairing functional poorly determined. Usually 1-2 terms active.

Mean-field equations

Mean-field potentials:

$$\begin{aligned}\Gamma_t^{\text{even}} &= -\vec{\nabla} \cdot M_t(\vec{r}) \vec{\nabla} + U_t(\vec{r}) + \frac{1}{2i} (\vec{\nabla} \sigma \cdot \vec{B}_t(\vec{r}) + \vec{B}_t(\vec{r}) \cdot \vec{\nabla} \sigma) \\ \Gamma_t^{\text{odd}} &= -\vec{\nabla} \cdot (\vec{\sigma} \cdot \vec{C}_t(\vec{r})) \vec{\nabla} + \vec{\sigma} \cdot \vec{\Sigma}_t(\vec{r}) + \frac{1}{2i} (\vec{\nabla} \cdot \vec{I}_t(\vec{r}) + \vec{I}_t(\vec{r}) \cdot \vec{\nabla}) - \vec{\nabla} \cdot \vec{D}_t(\vec{r}) \vec{\sigma} \cdot \vec{\nabla}\end{aligned}$$

where

$$\begin{aligned}U_t &= 2C_t^\rho \rho_t + 2C_t^{\Delta\rho} \Delta\rho_t + C_t^\tau \tau_t + C_t^{\nabla J} \vec{\nabla} \cdot \vec{J}_t, \\ \vec{\Sigma}_t &= 2C_t^s \vec{s}_t + 2C_t^{\Delta s} \Delta\vec{s}_t + C_t^T \vec{T}_t + C_t^{\nabla j} \vec{\nabla} \times \vec{j}_t, -2C_t^{\nabla s} \Delta\vec{s}_t + C_t^F \vec{F}_t - 2C_t^{\nabla s} \vec{\nabla} \times (\vec{\nabla} \times \vec{s}_t) \\ M_t &= C_t^\tau \rho_t, \\ \vec{C}_t &= C_t^T \vec{s}_t, \\ \vec{B}_t &= 2C_t^J \vec{J}_t - C_t^{\nabla J} \vec{\nabla} \rho_t, \\ \vec{I}_t &= 2C_t^j \vec{j}_t + C_t^{\nabla j} \vec{\nabla} \times \vec{s}_t, \\ \vec{D}_t &= C_t^F \vec{s}_t,\end{aligned}$$

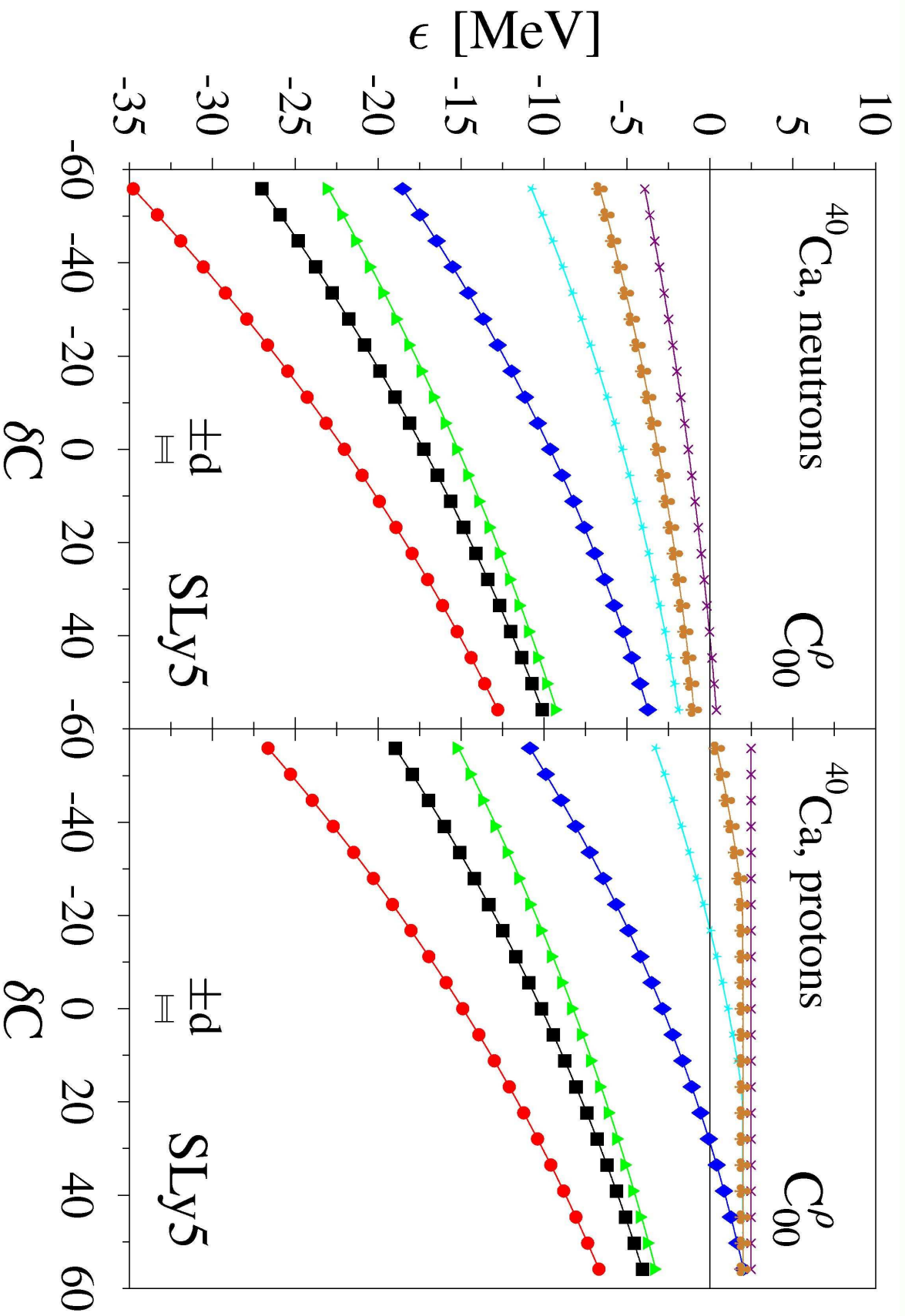
Neutron and proton mean-field Hamiltonians:

$$\begin{aligned}h_n &= -\frac{\hbar^2}{2m} \Delta + \Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} + \Gamma_1^{\text{even}} + \Gamma_1^{\text{odd}}, \\ h_p &= -\frac{\hbar^2}{2m} \Delta + \Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} - \Gamma_1^{\text{even}} - \Gamma_1^{\text{odd}}.\end{aligned}$$

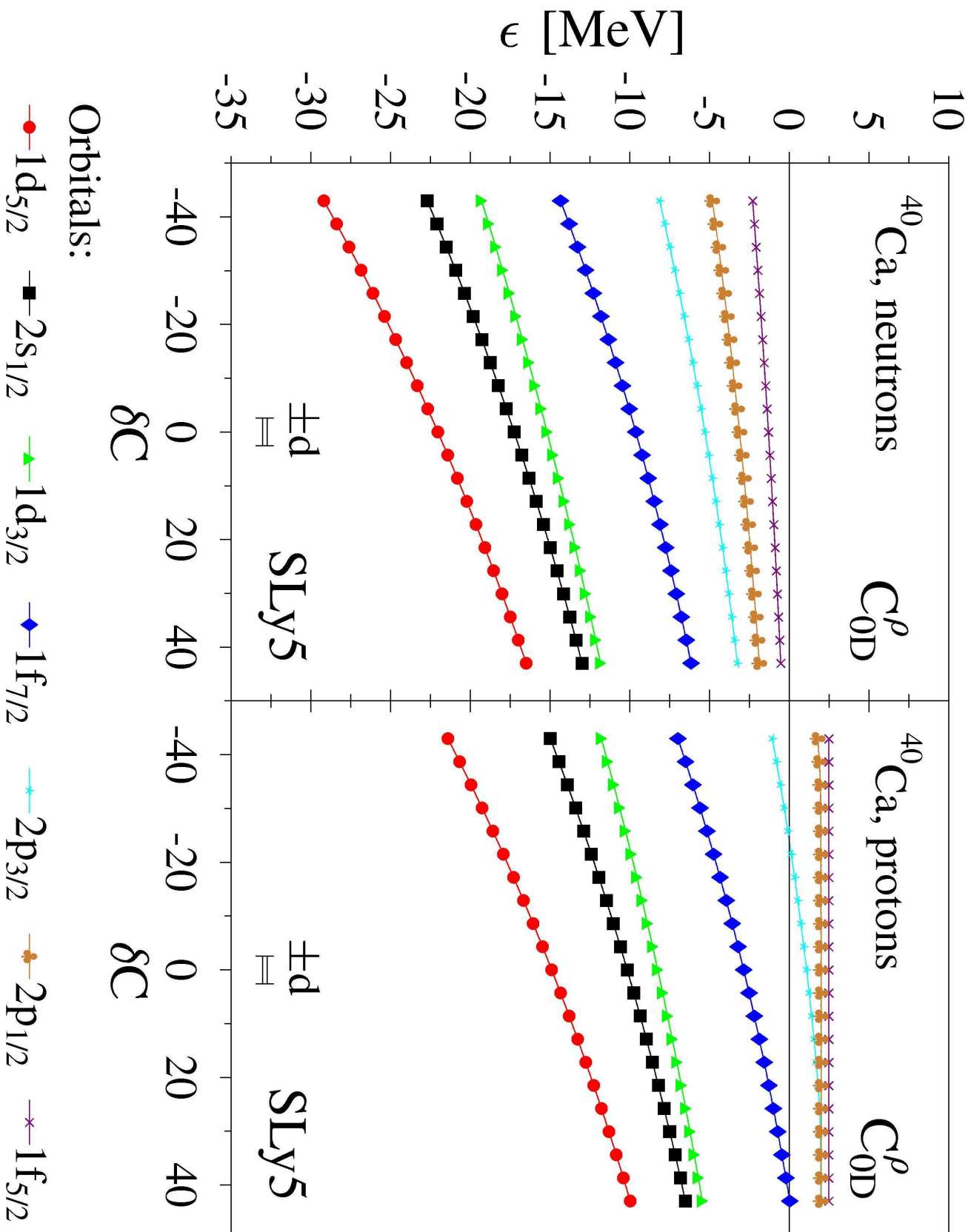
HF equation for single-particle wave functions:

$$h_\alpha \psi_{i,\alpha}(\vec{r}\sigma) = \epsilon_{i,\alpha} \psi_{i,\alpha}(\vec{r}\sigma),$$

where i numbers the neutron ($\alpha=n$) and proton ($\alpha=p$) eigenstates.

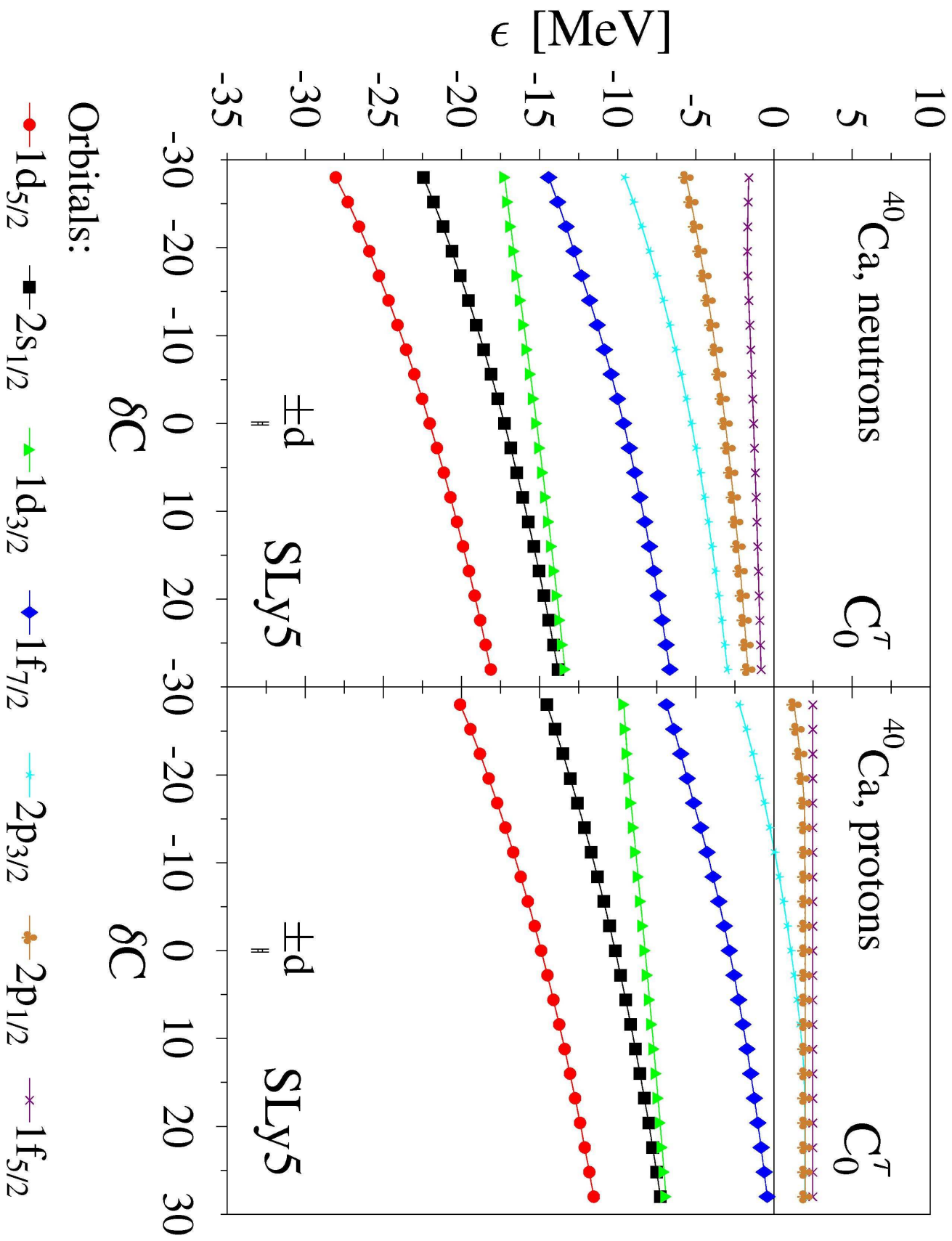


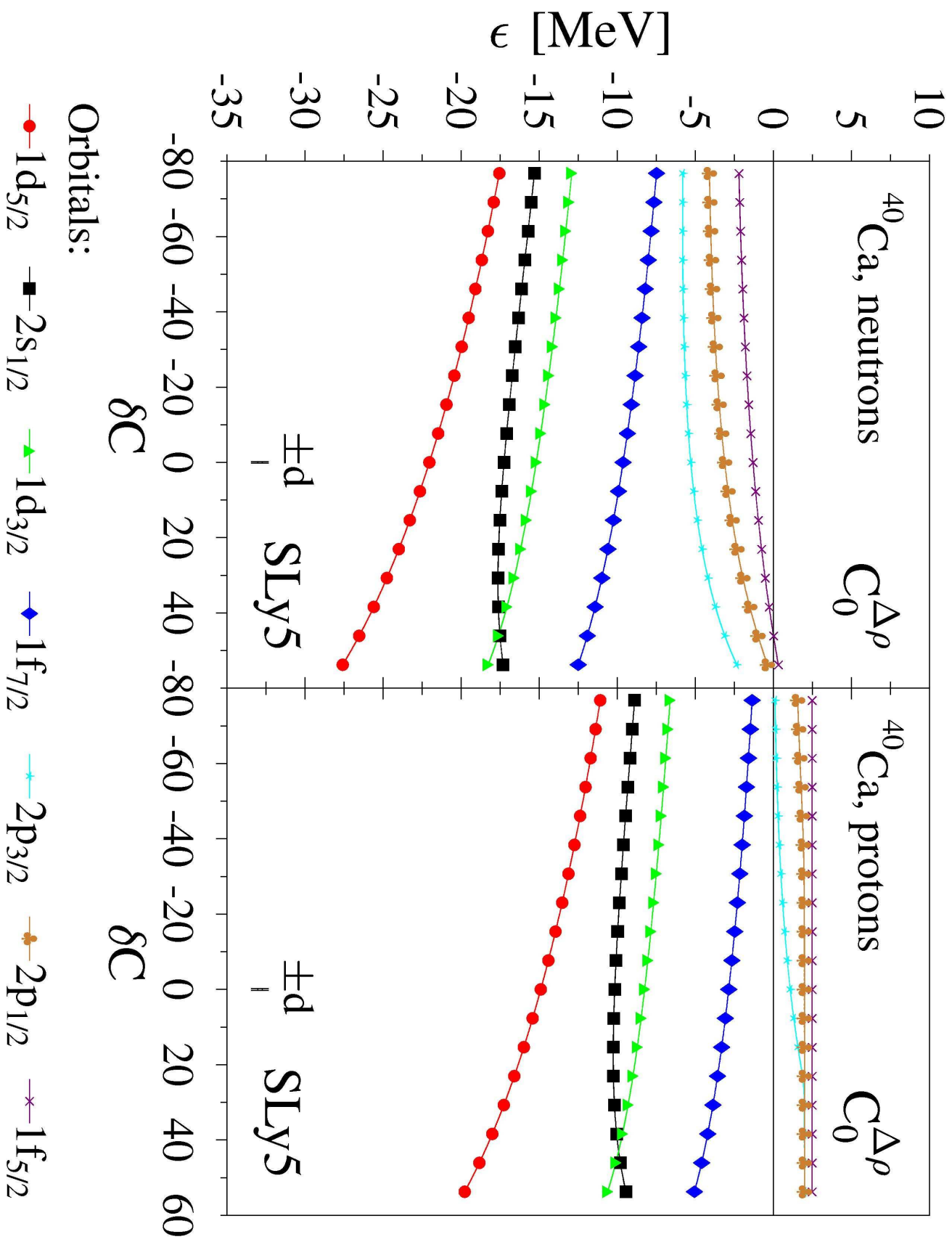
M. Kortelainen et al., arXiv:0803.2291

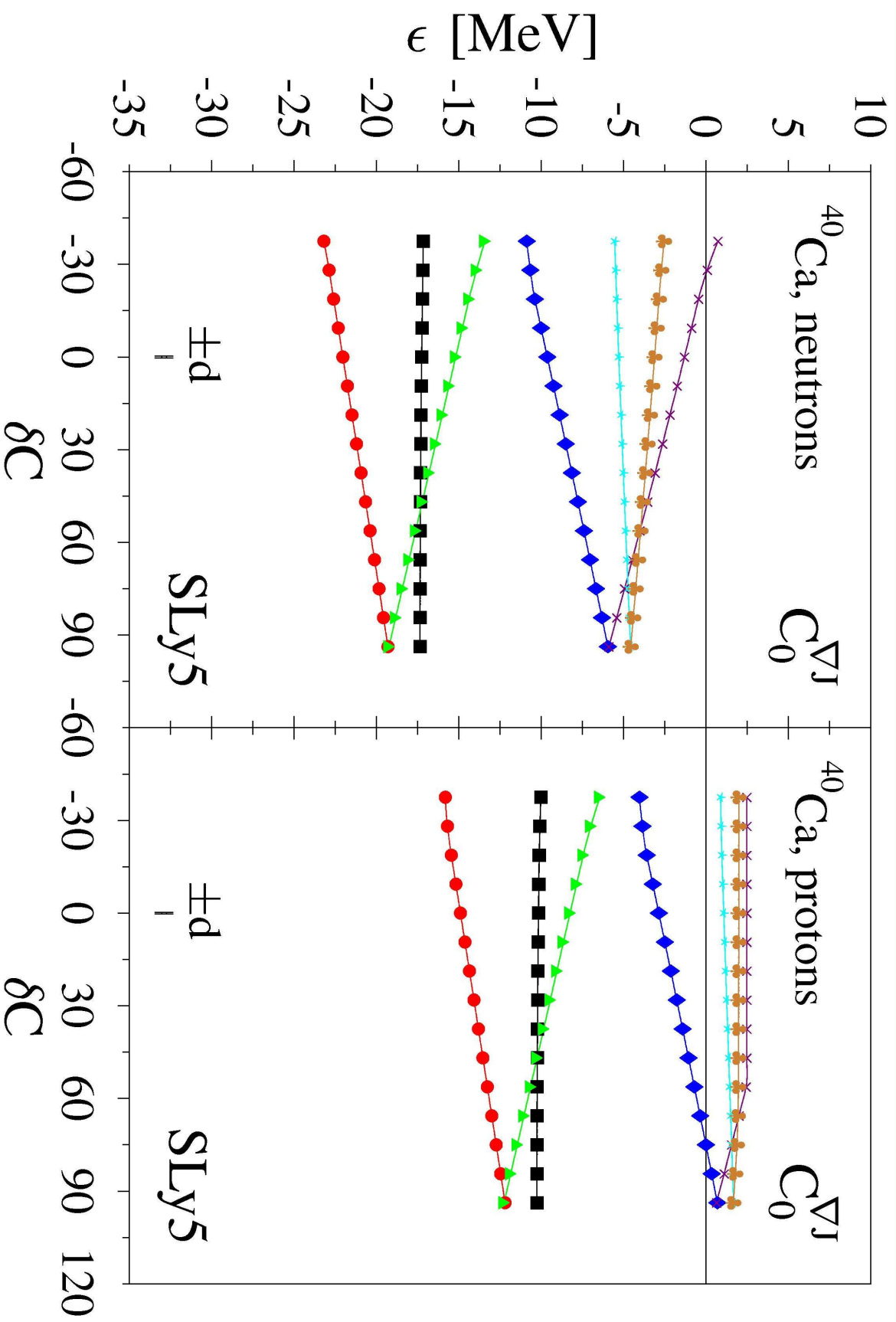


Orbitals:

- $1d_{5/2}$
- $2s_{1/2}$
- ▲ $1d_{3/2}$
- ◆ $1f_{7/2}$
- ✦ $2p_{3/2}$
- ✪ $2p_{1/2}$
- ✱ $1f_{5/2}$







M. Kortelainen et al., arXiv:0803.2291

Linear Regression Analysis

Derivatives of single-particle energies with respect to coupling constants β_{im} can be calculated in several ways.

1° The Feynman-Hellman theorem:

$$\beta_{im} = \langle \phi_i | \frac{\partial h}{\partial C_m} | \phi_i \rangle,$$

2° Finite-difference approximation:

$$\beta_{im} = \frac{\partial \epsilon_i}{\partial C_m}(C_m^0) \simeq \frac{\epsilon_i(C_m^+) - \epsilon_i(C_m^-)}{C_m^+ - C_m^-},$$

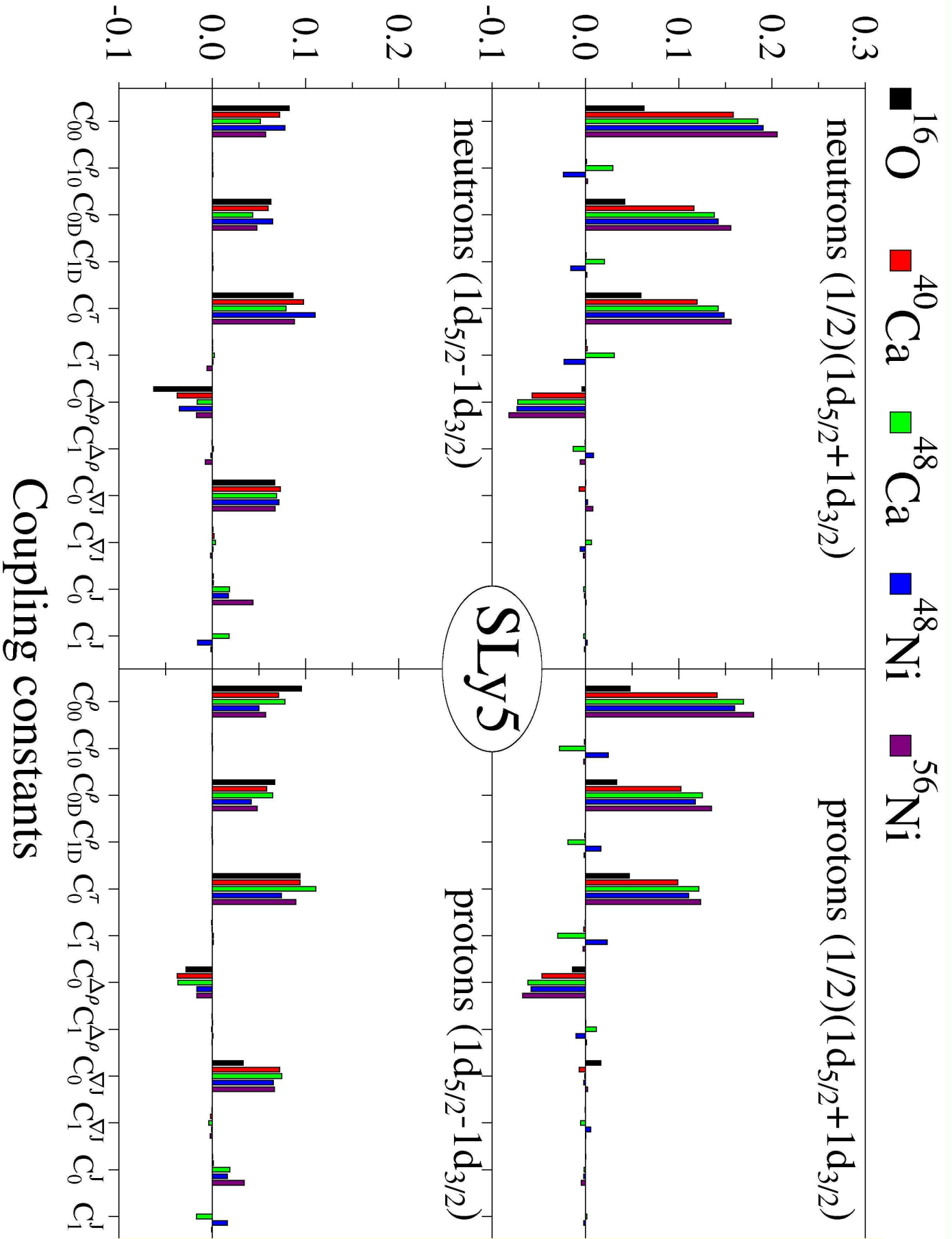
3° Linear Regression Analysis:

$$\epsilon_i(C_m^0 + d_m^k) = \beta_{im} d_m^k + \beta_i^0 + r_i^k,$$

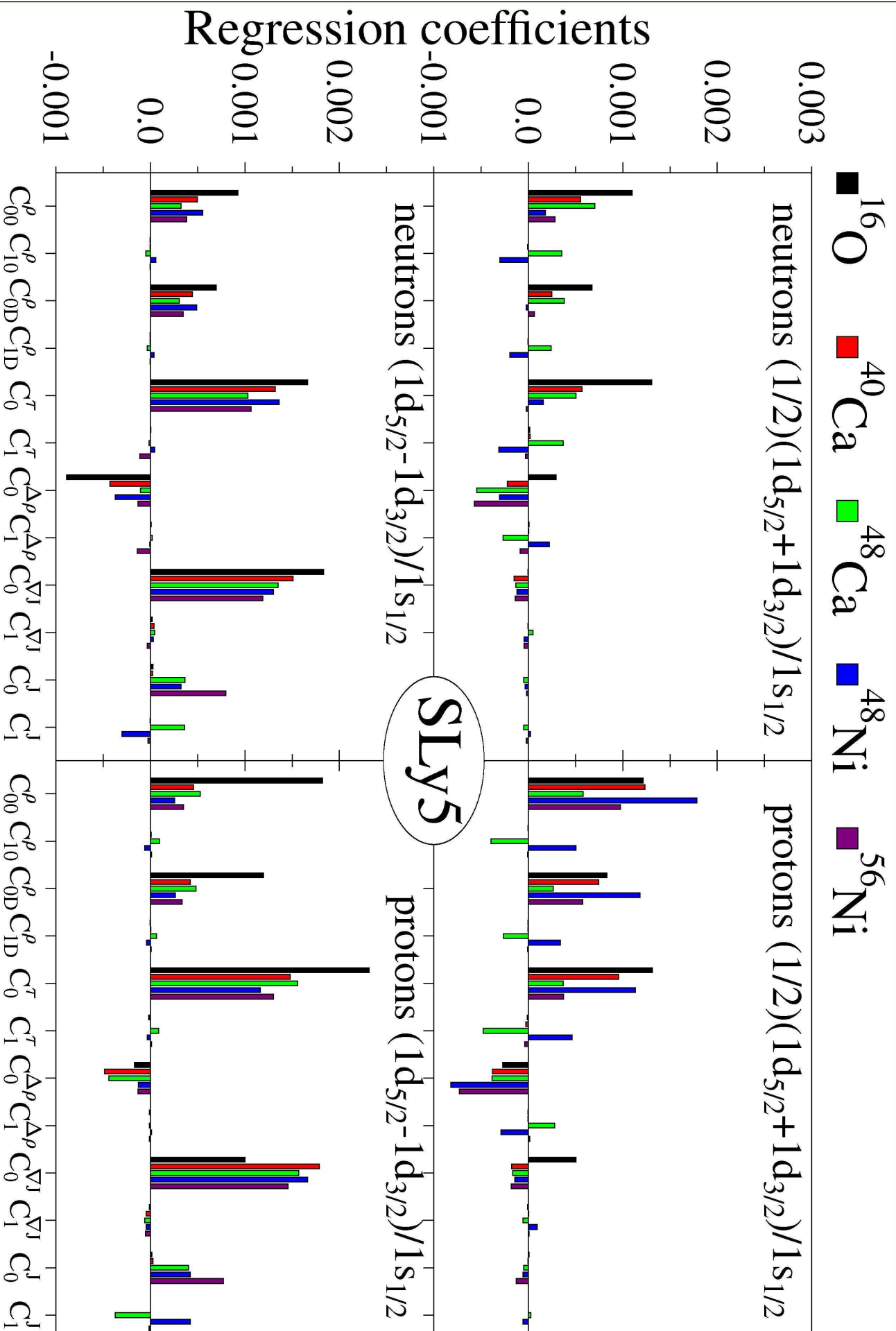
Instead of analyzing the s.p. energies we may equivalently look at the centroids of SO partners and their SO splittings:

$$\begin{aligned} \epsilon_{nl}^{\text{cent}} &= \frac{1}{2} (\epsilon_{nlj<} + \epsilon_{nlj>}), \\ \epsilon_{nl}^{\text{SO}} &= \epsilon_{nlj<} - \epsilon_{nlj>}, \end{aligned}$$

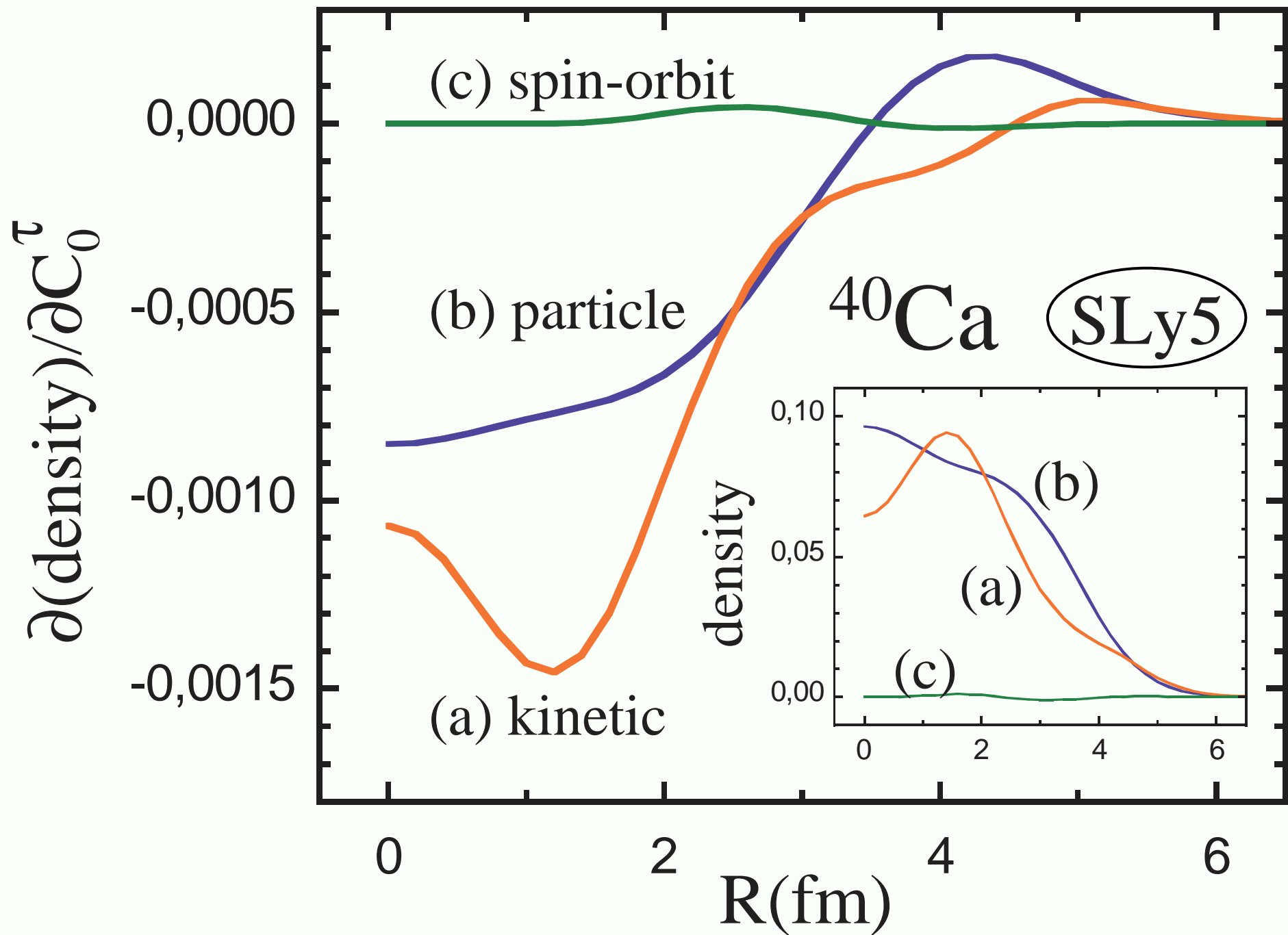
Regression coefficients



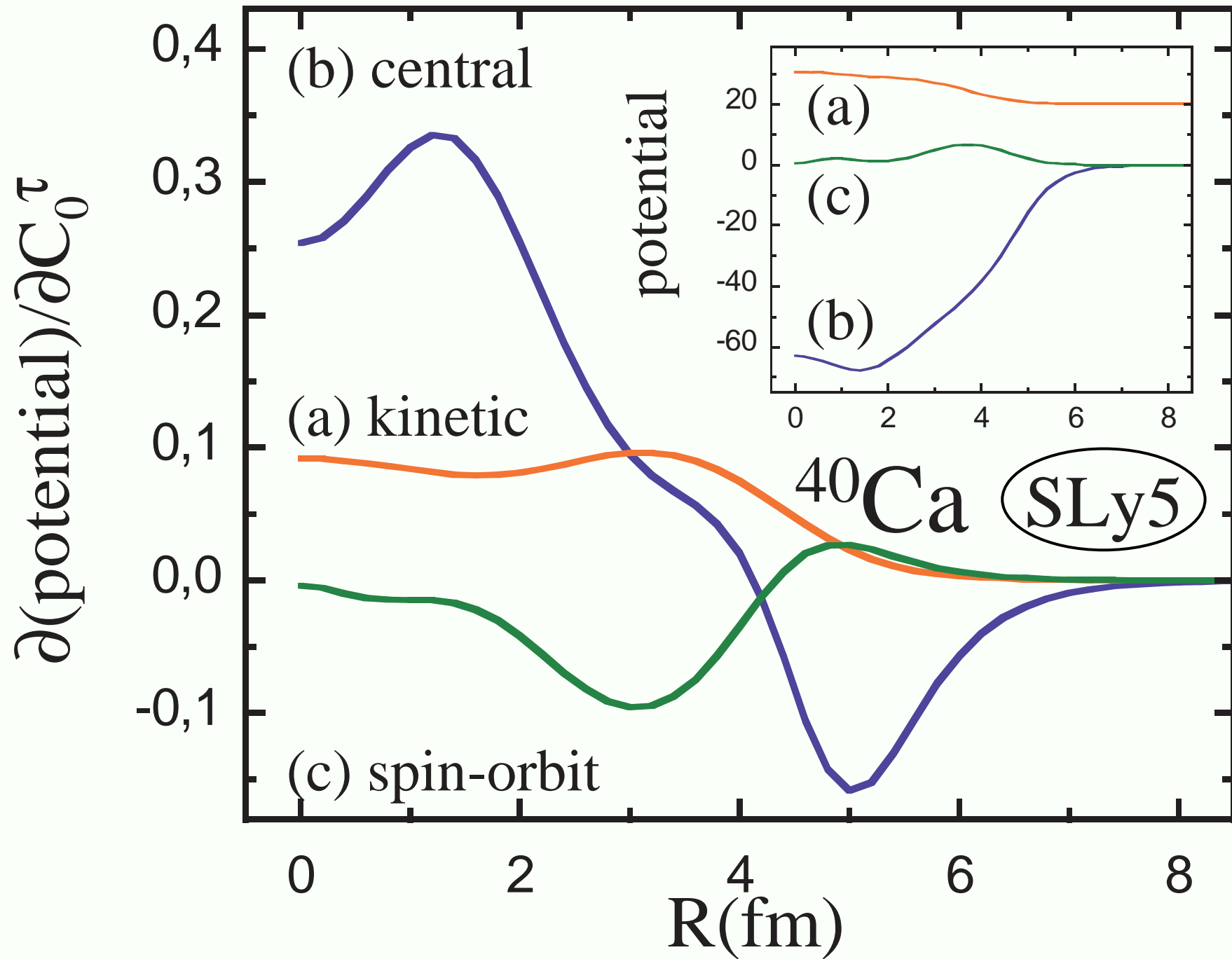
M. Kortelainen et al., arXiv:0803.2291



M. Kortelainen et al., arXiv:0803.2291

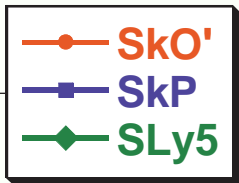
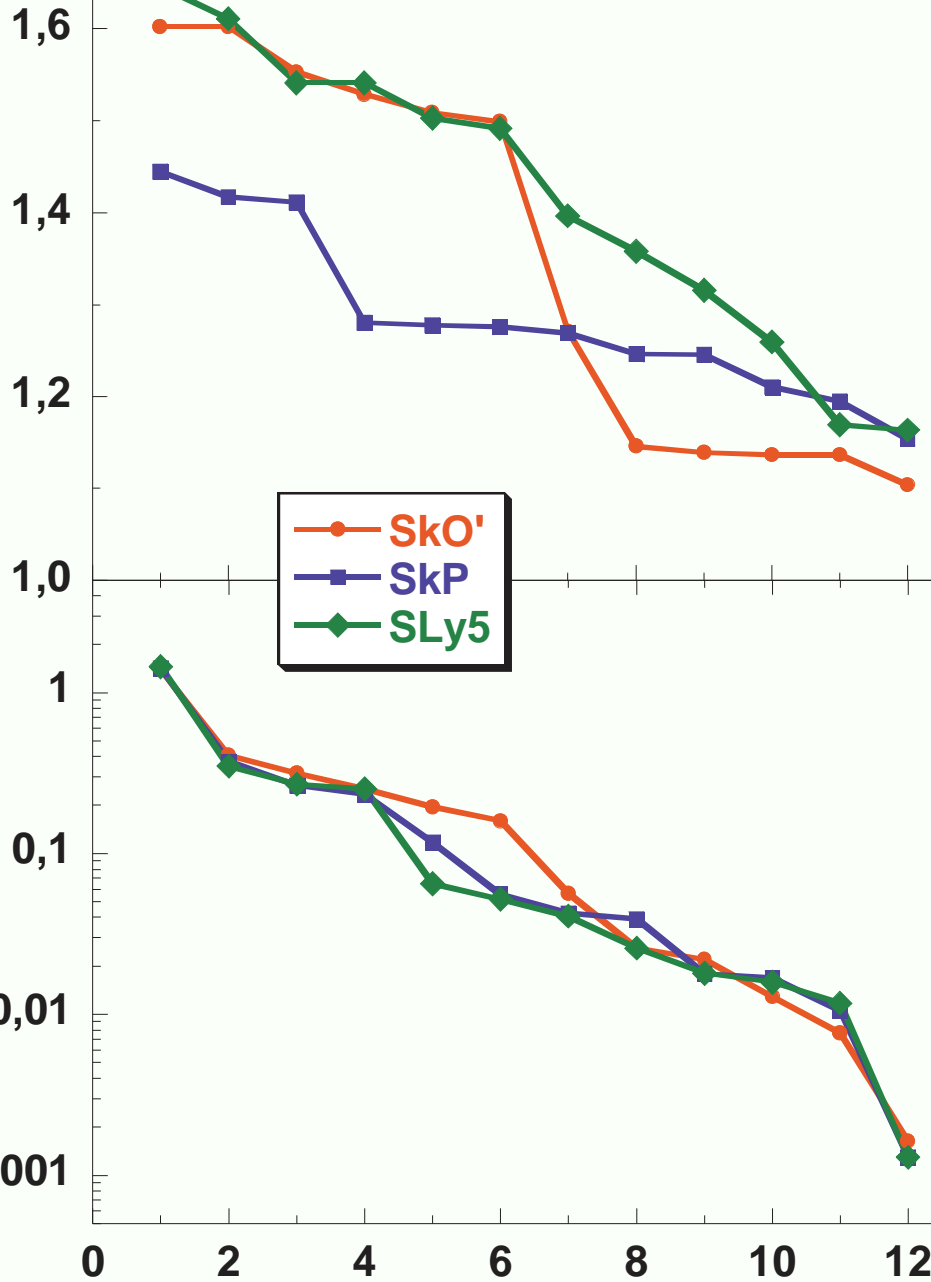


M. Kortelainen et al., arXiv:0803.2291

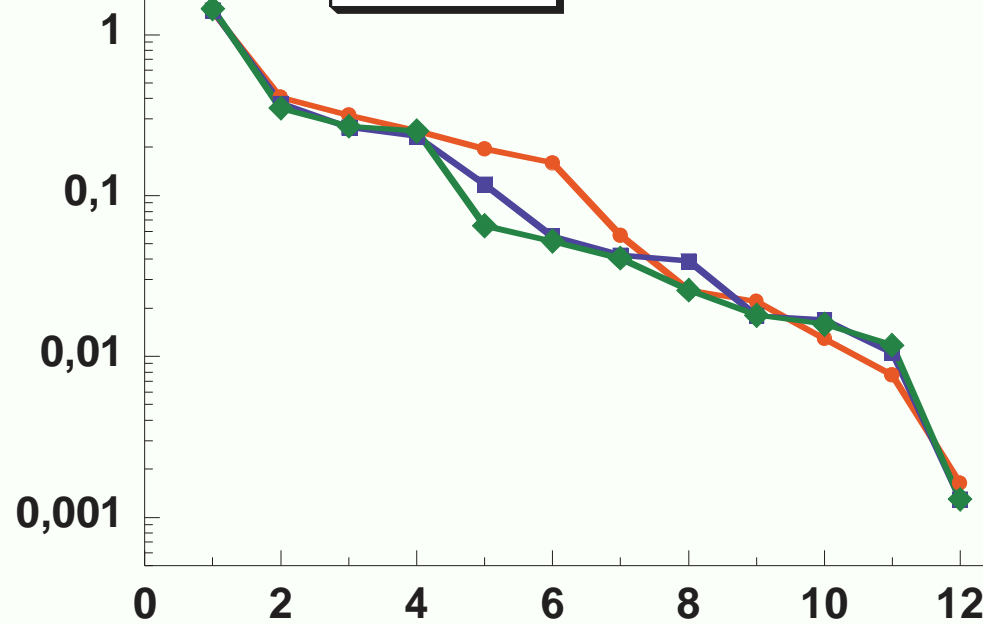


M. Kortelainen et al., arXiv:0803.2291

RMS deviation of
s.p. energies (MeV)



Singular value



Number of singular value

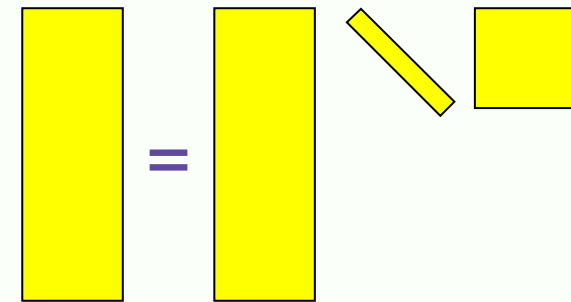
Fits of s.p. energies

$$\epsilon_i - \epsilon_i^{\text{exp}} = -\sum_m \beta_{im} \Delta C_m,$$

EXP: M.N. Schwierz, I. Wiedenhover,
and A. Volya, arXiv:0709.3525

Singular value decomposition

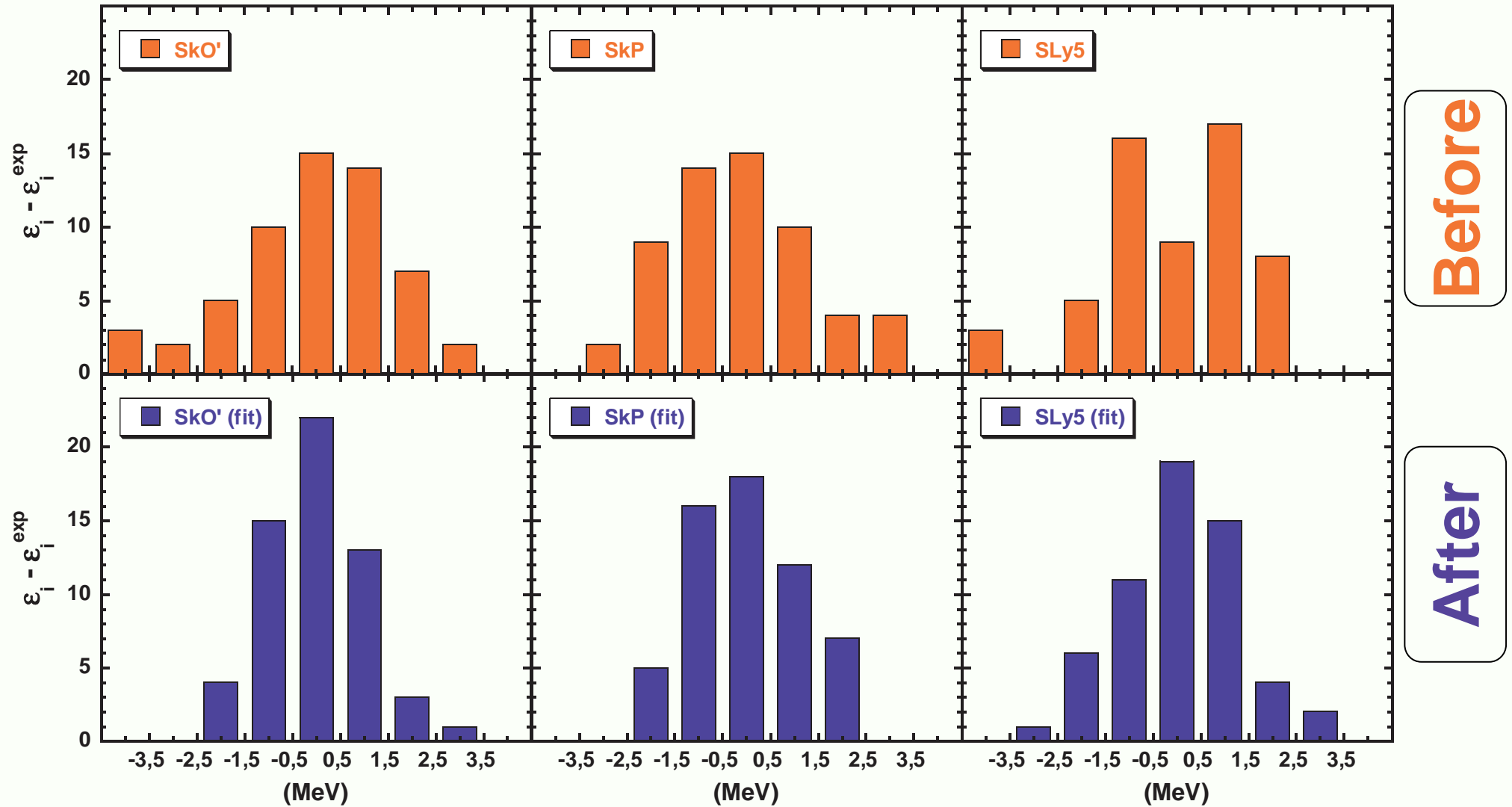
$$\beta_{im} = \sum_{\mu} V_{i\mu} d_{\mu} U_{\mu m}^T,$$



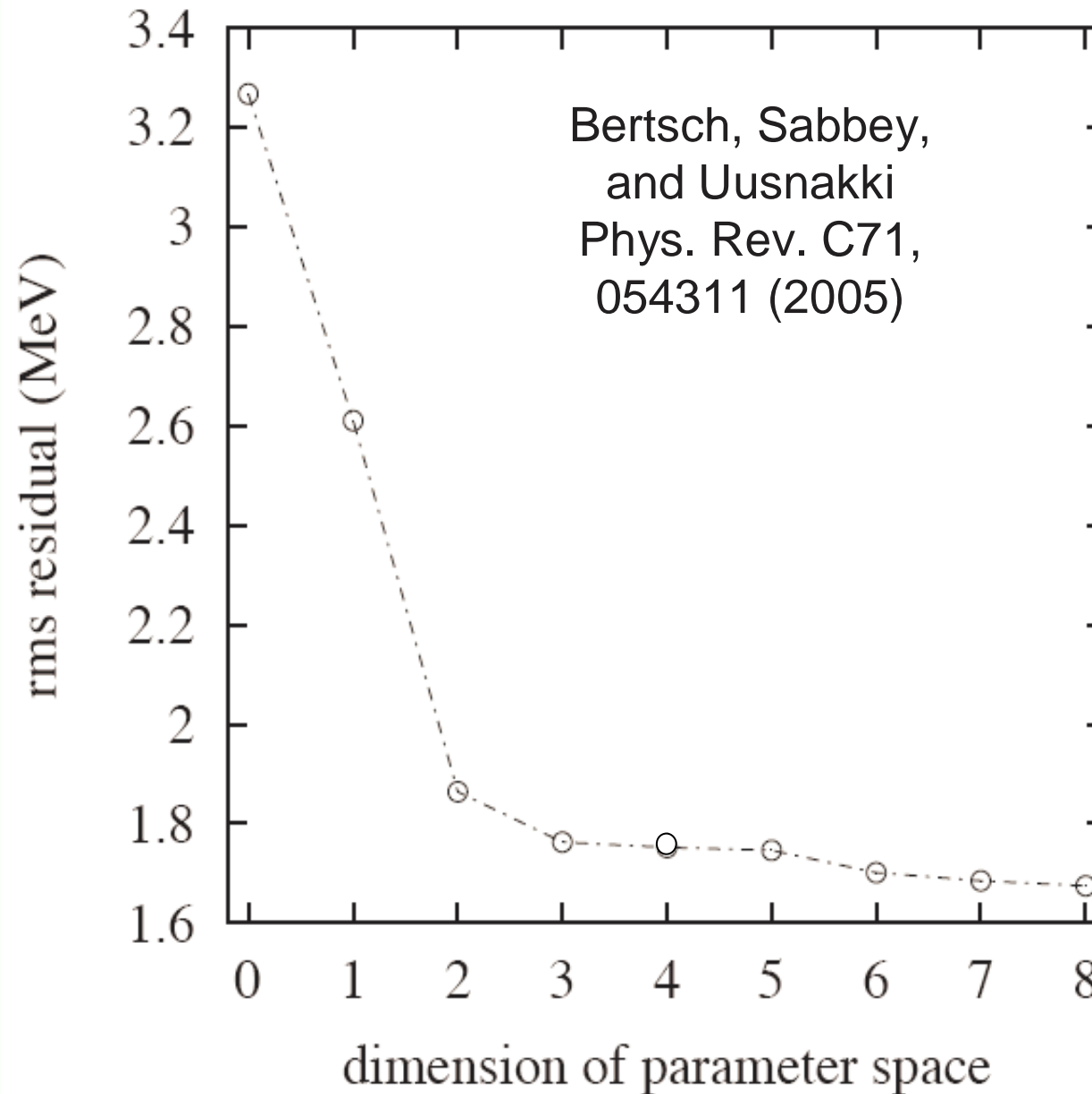
$$\sum_i V_{i\mu} V_{i\nu} = \delta_{\mu\nu},$$

$$\sum_m U_{m\mu} U_{m\nu} = \delta_{\mu\nu},$$

Fits of single-particle energies



How many parameters are really needed?

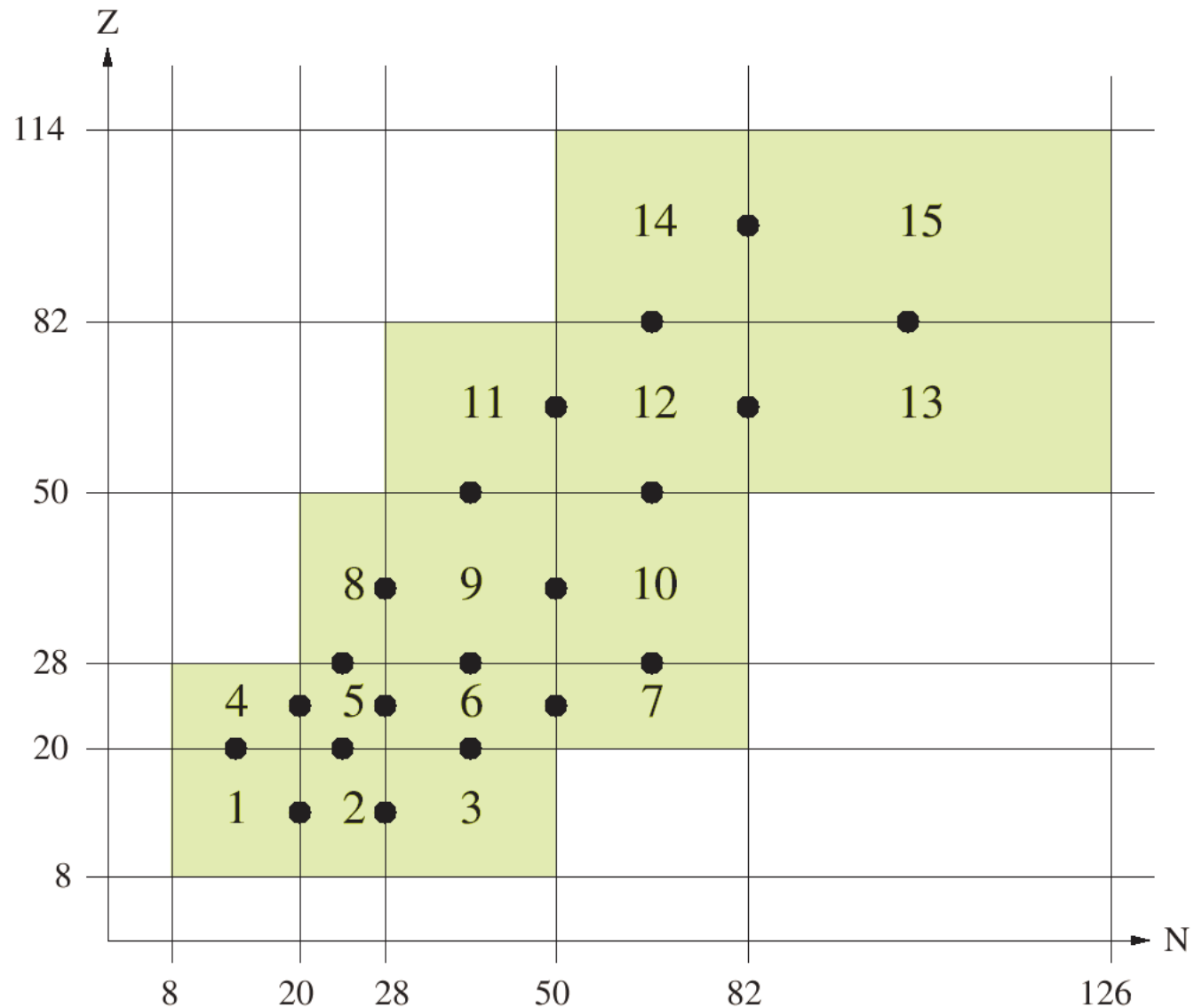


Witek
19 marca 2008

Global (masses)

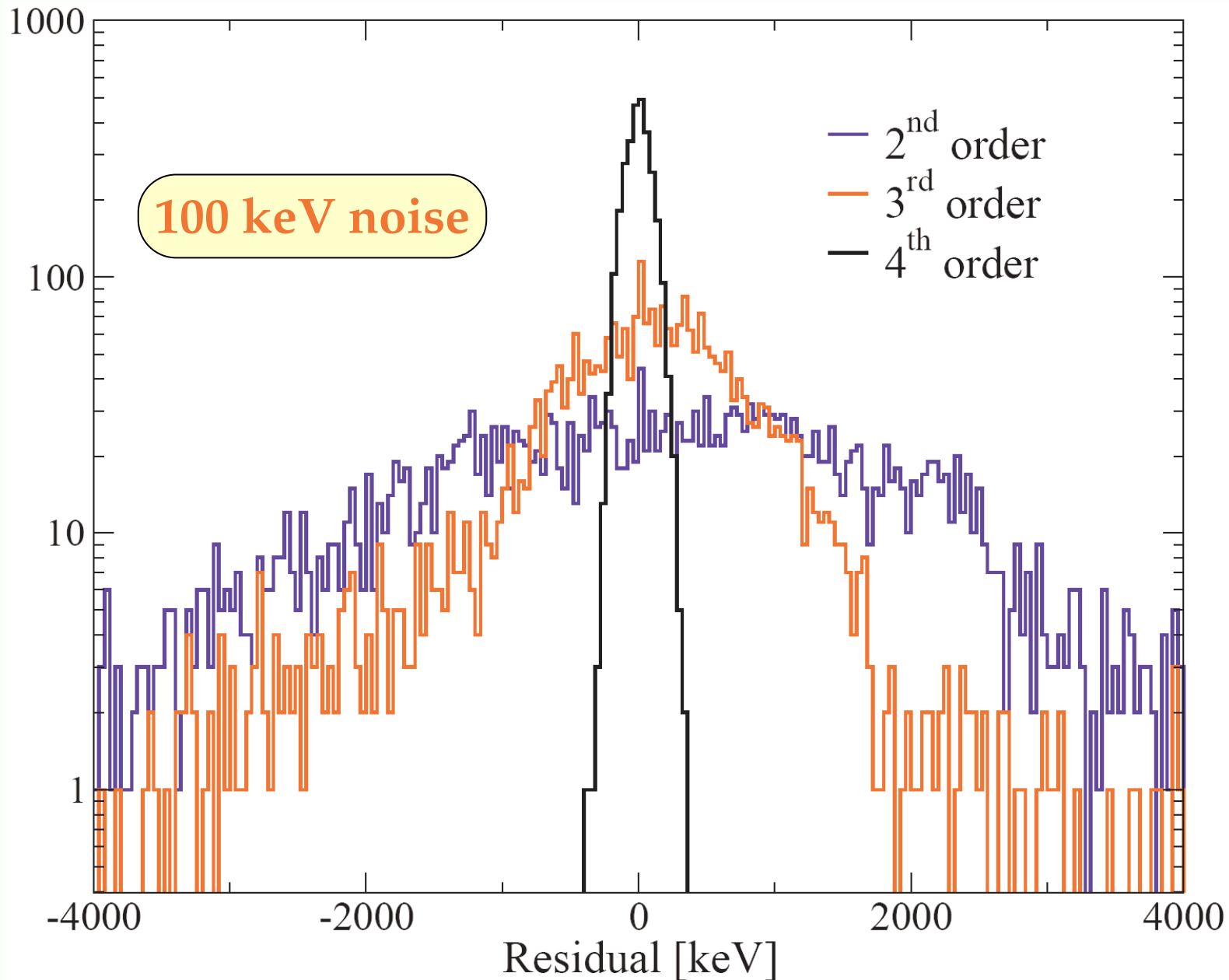
A simple model to produce nuclear-mass metadata

- Liquid-drop model
- 4th order polynomial in each of the 15 regions between the magic numbers
- Gaussian noise



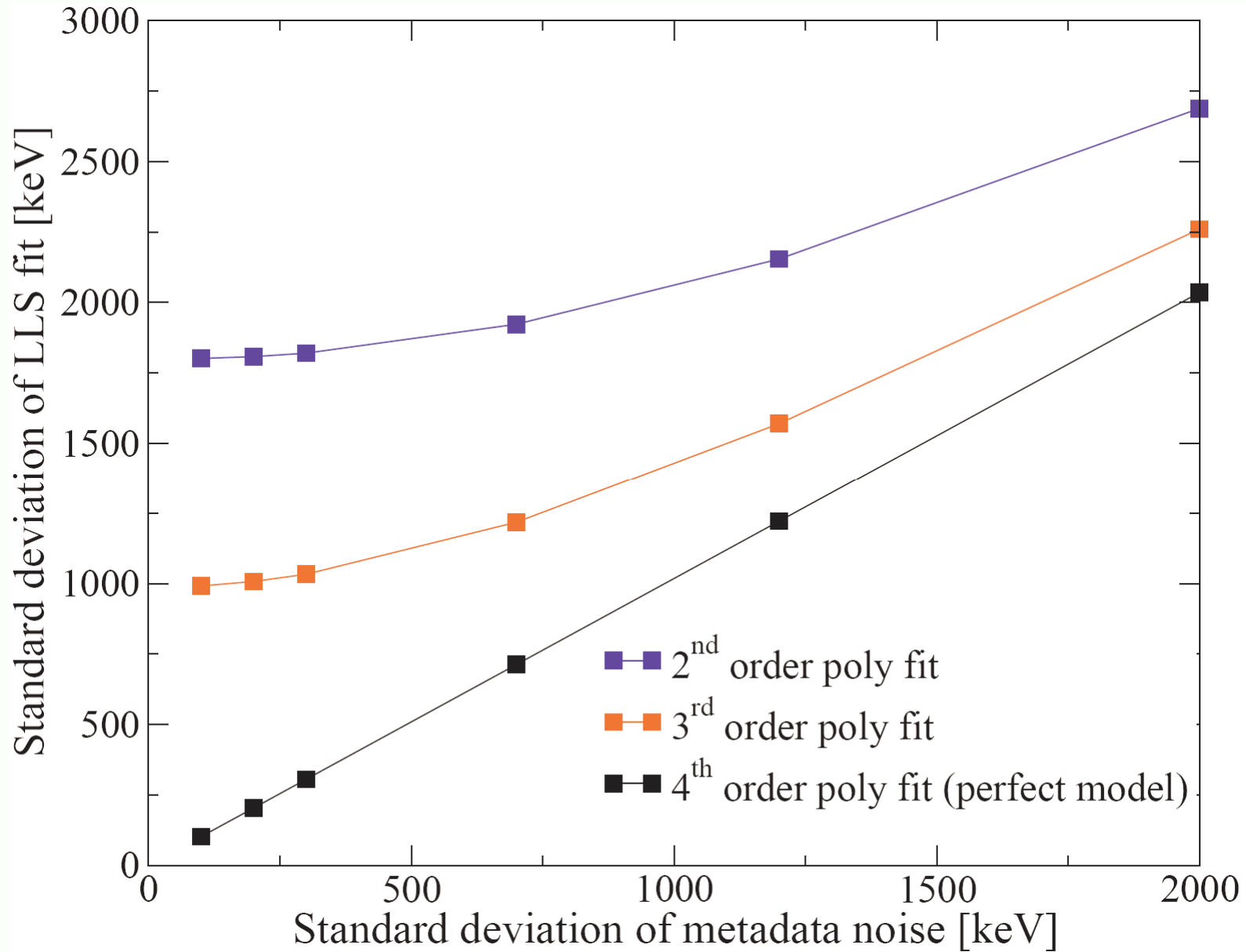
J. Toivanen et al., to be published

Distribution of residuals



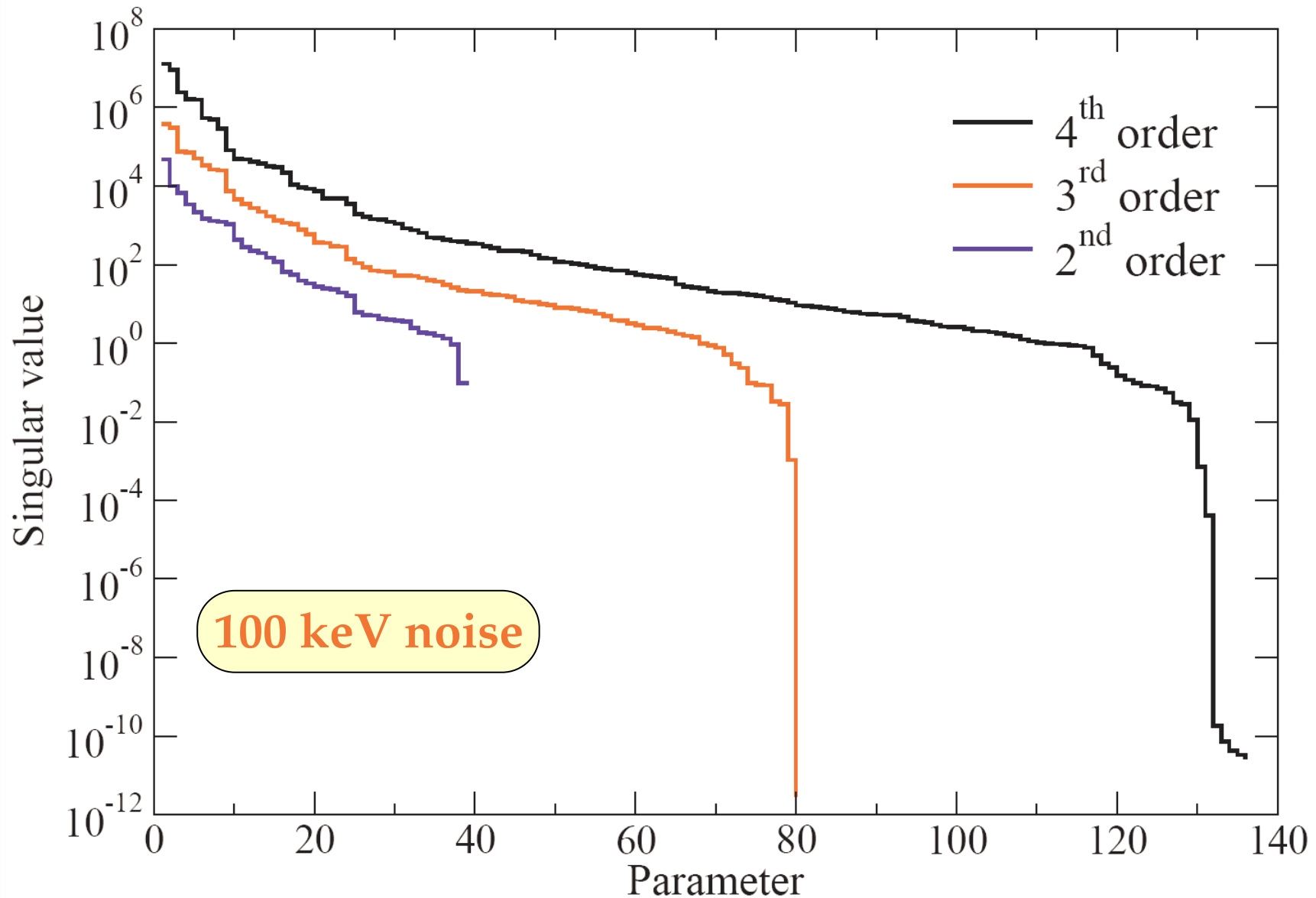
J. Toivanen et al., to be published

Dependence of standard deviations on the noise



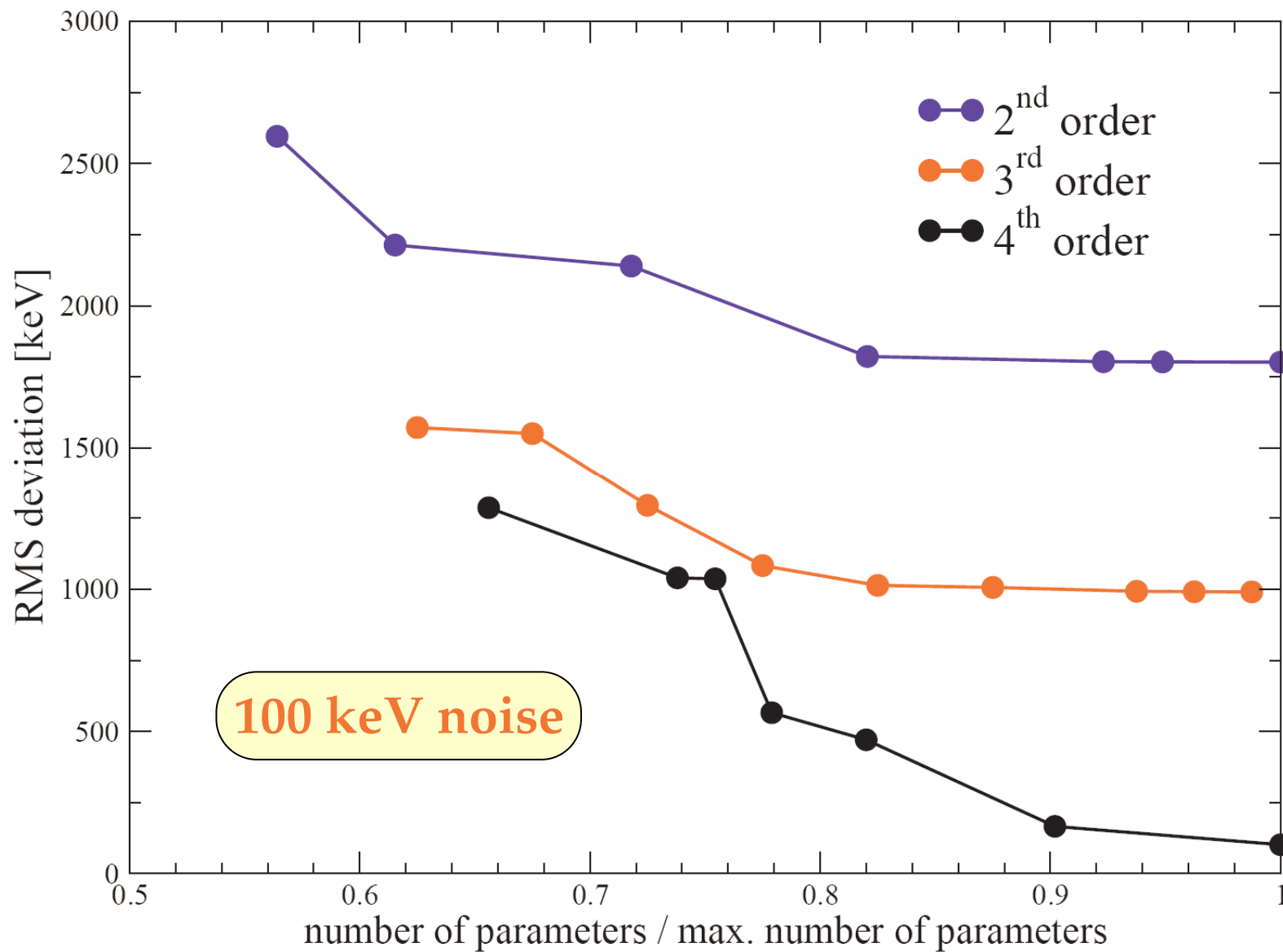
J. Toivanen *et al.*, to be published

Distribution of singular values



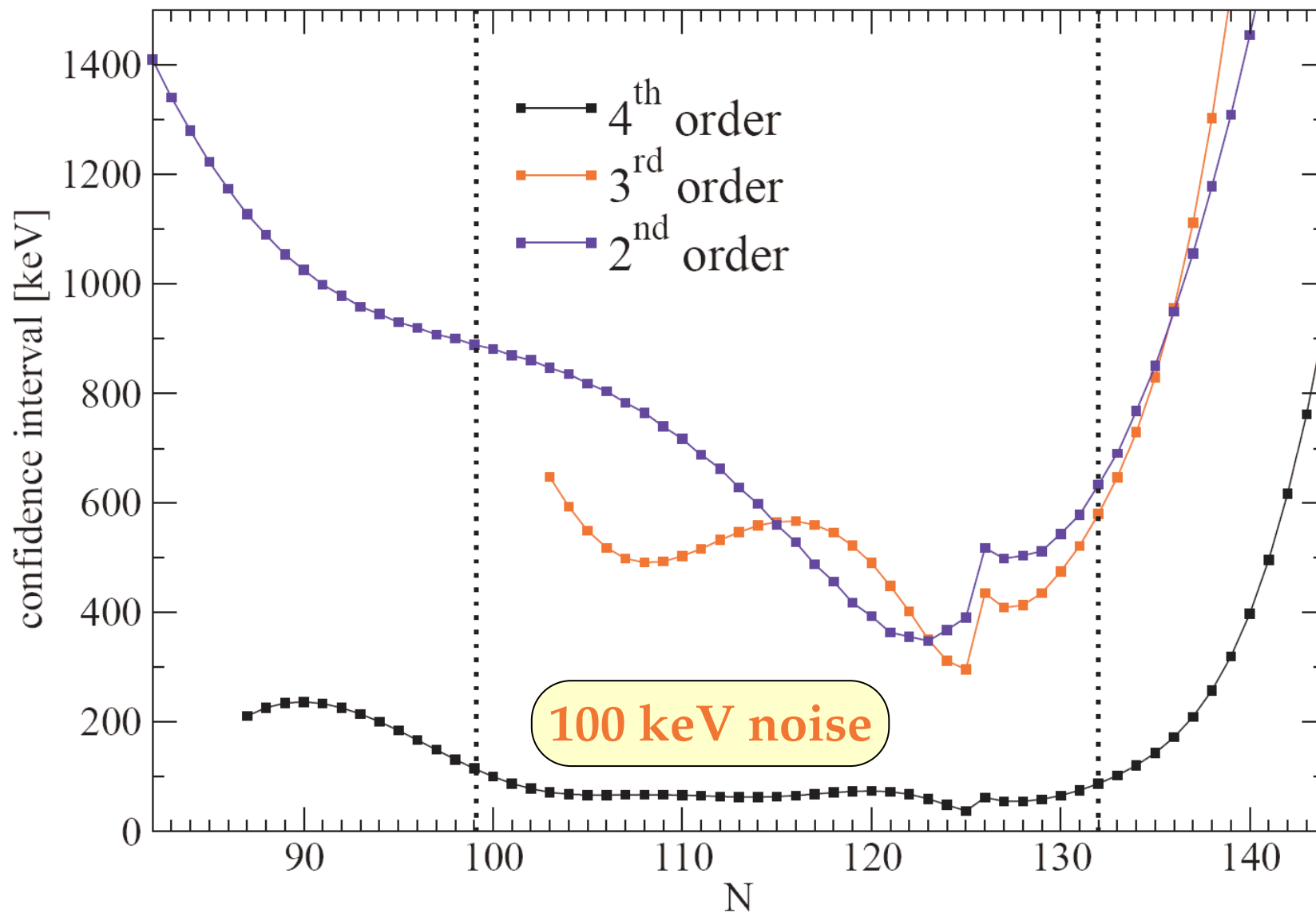
J. Toivanen et al., to be published

Dependence of standard deviations on the number of parameters



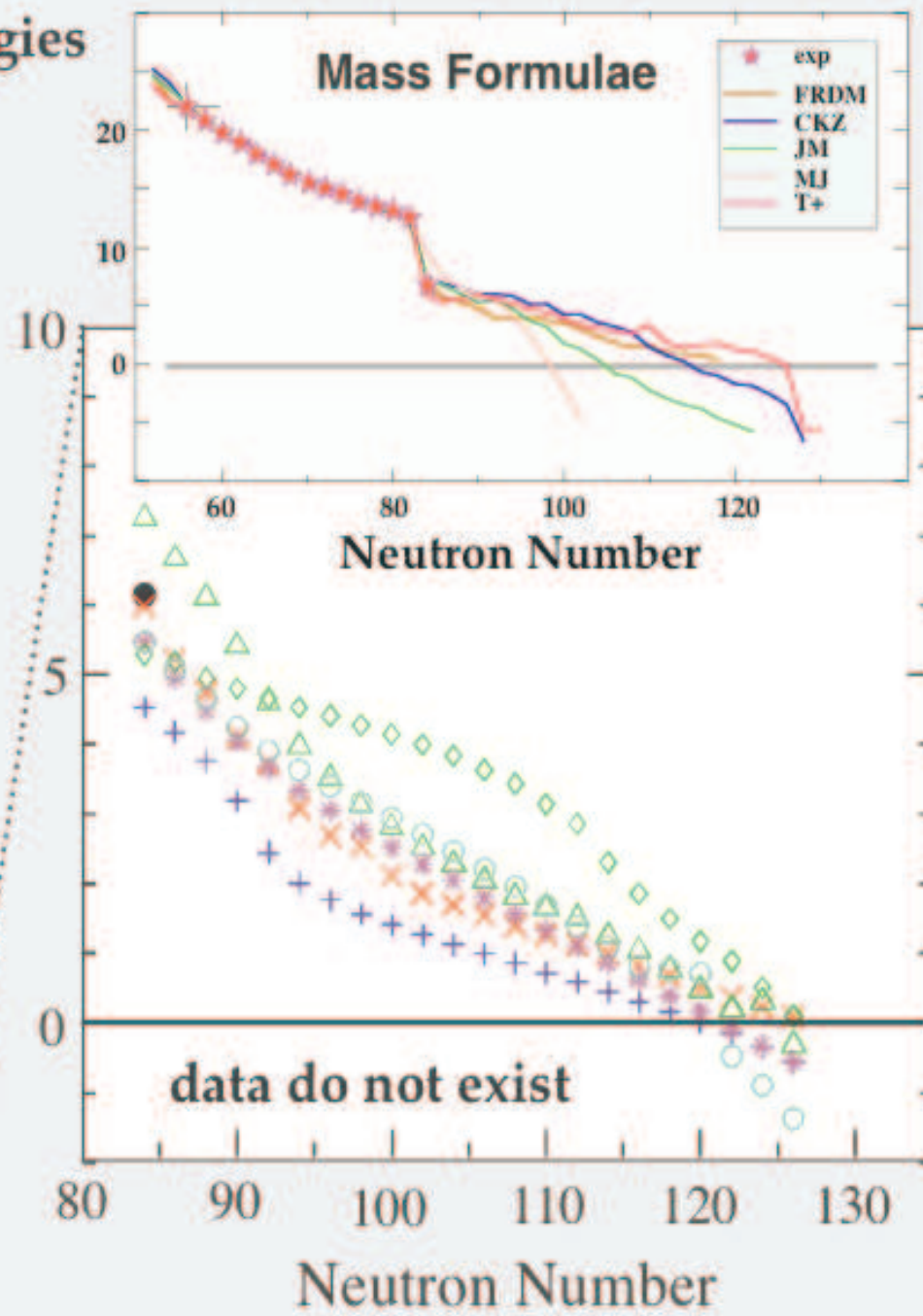
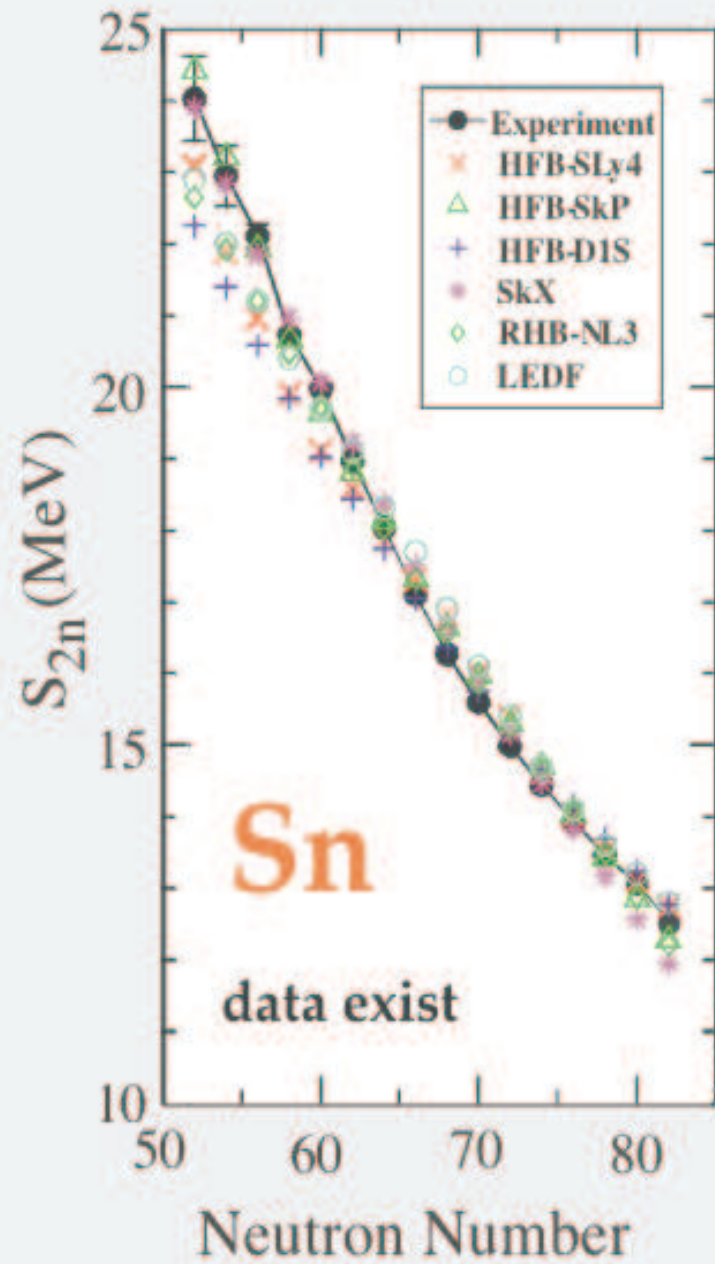
J. Toivanen et al., to be published

Error propagation



J. Toivanen et al., to be published

two-neutron separation energies



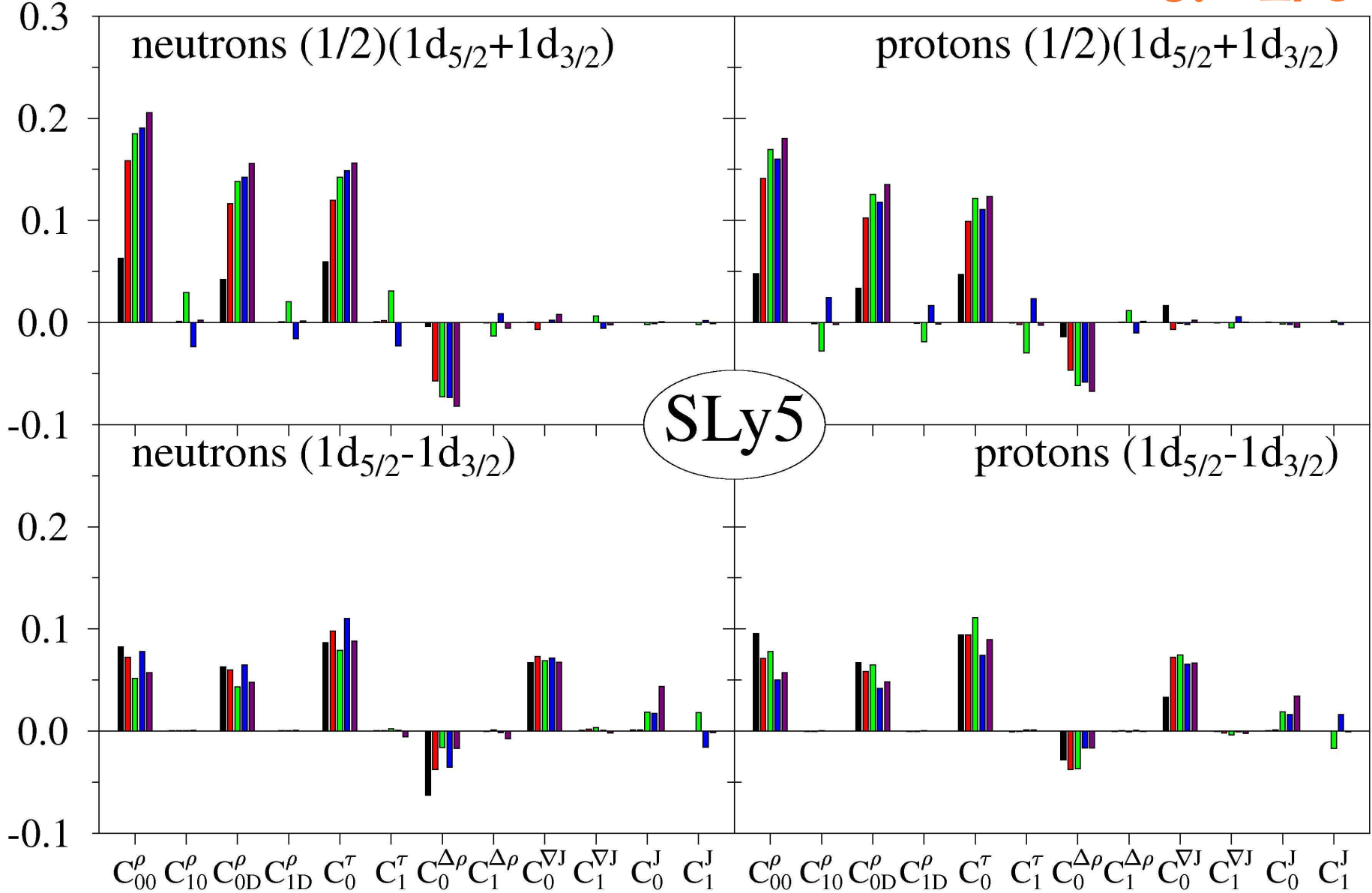
Podsumowanie i wnioski

1. Teoria funkcjonału gęstości oparta jest na silnych ale niekonstruktywnych twierdzeniach mechaniki kwantowej.
2. Konstrukcja jądrowego funkcjonału gęstości oparta jest na szczególnych przesłankach fizycznych.
3. Energie jednocząstkowe (jak również masy całkowite) zależą w przybliżeniu liniowo od stałych sprzężenia.
4. Standardowa parametryzacja jądrowego funkcjonału gęstości:
 - nie pozwala na pełne rozdzielenie efektów rozszczepienia spin-orbita od masy efektywnej,
 - nie jest wystarczająco bogata aby poprawnie opisać doświadczalne energie jednocząstkowe.
5. Standardową parametryzację można rozszerzać poprzez bogatszą zależność stałych sprzężenia od gęstości, uwzględnienie wyższych niż druga pochodnych gęstości i/lub uwzględnienie wyższych niż druga potęg gęstości.
6. Profesjonalna analiza błędów jest niezbędnym elementem działalności teoretyka.

■ ^{16}O
 ■ ^{40}Ca
 ■ ^{48}Ca
 ■ ^{48}Ni
 ■ ^{56}Ni

$\alpha=1/6$

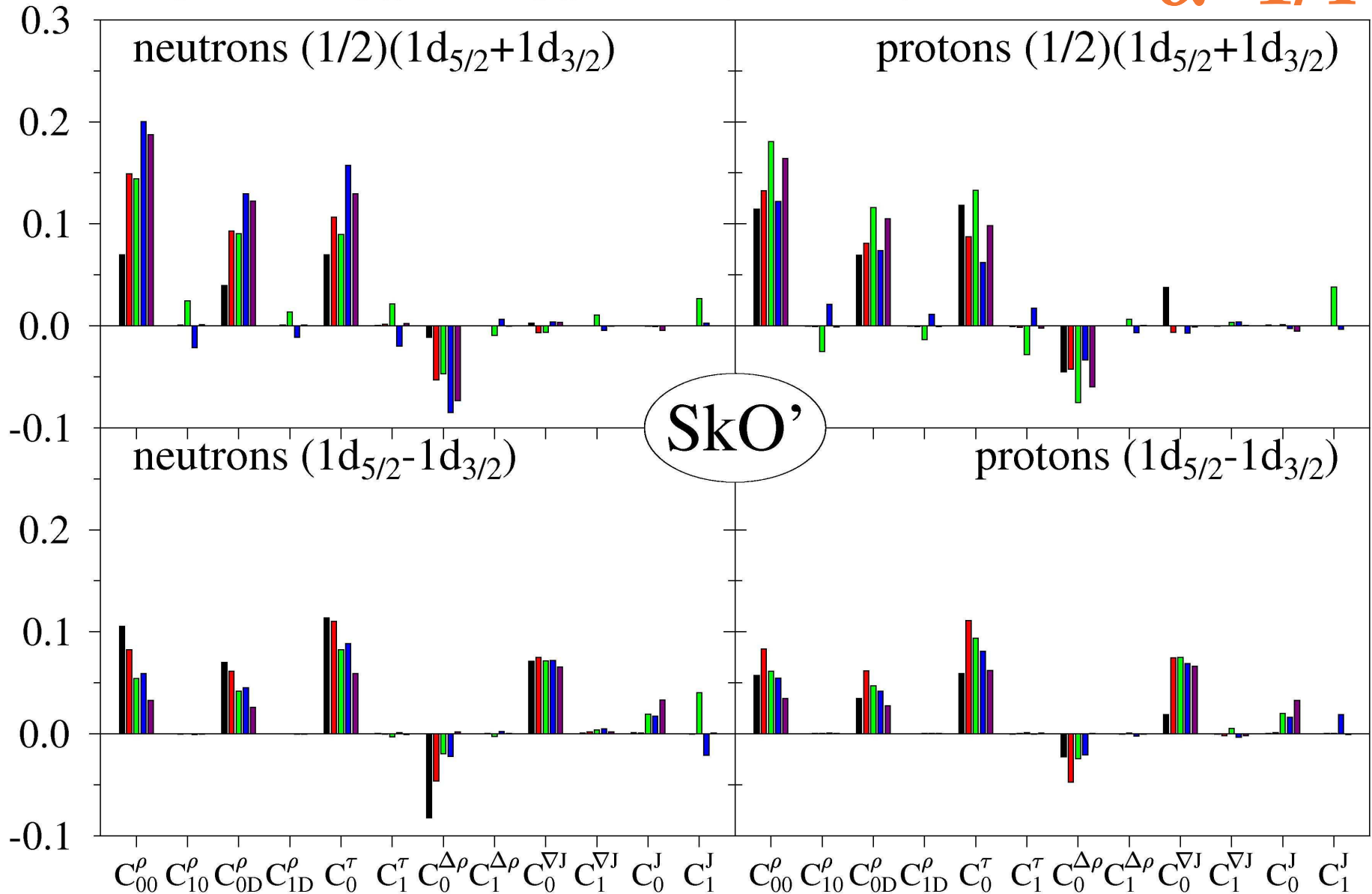
Regression coefficients



■ ^{16}O
 ■ ^{40}Ca
 ■ ^{48}Ca
 ■ ^{48}Ni
 ■ ^{56}Ni

$\alpha=1/4$

Regression coefficients

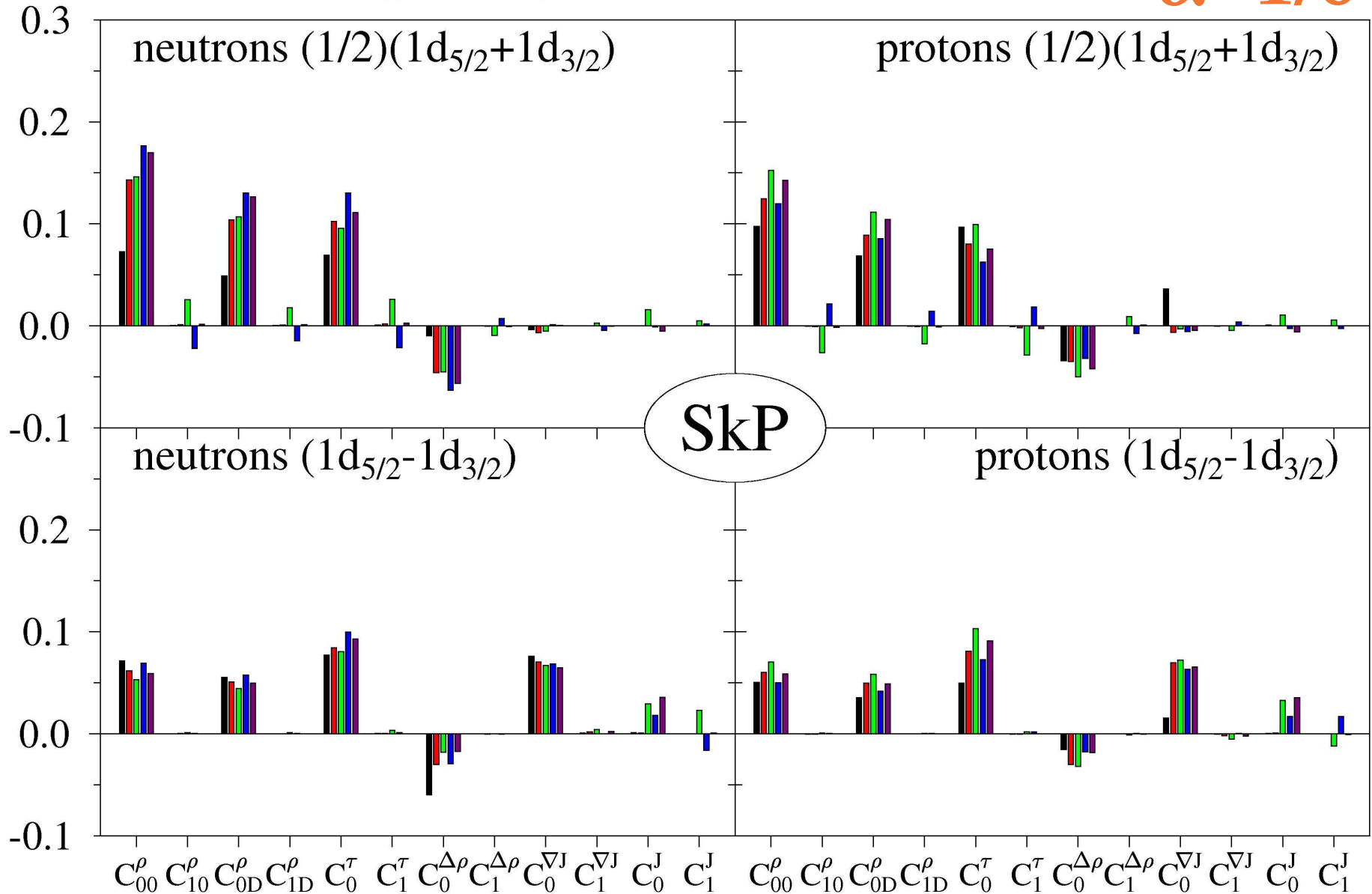


Coupling constants

■ ^{16}O
 ■ ^{40}Ca
 ■ ^{48}Ca
 ■ ^{48}Ni
 ■ ^{56}Ni

$\alpha=1/6$

Regression coefficients



Coupling constants